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Abstract

A random walk in a discrete space of large dimensions is devised to find the free energy of finite Ising spin systems with nearest neighbor interactions. The system studied is the three dimensional cubic lattice, finite and periodic in two of the dimensions, and infinite in the third dimension. The effect of low-order surface terms in the graphical expansion of the free energy is shown by removing them from the numerical results for the finite lattice, and comparing this reduced free energy to the bulk free energy. Using transfer matrix formalism, a Monte Carlo solution is obtained by establishing a correspondence between the eigenvalue equation satisfied by the transfer matrix, and the collision density equation of the random walk. The walk is then simulated to provide Monte Carlo estimates of the free energy, magnetization, and spin correlation.

I. Introduction

One important area of investigation in physics at the present time is that of cooperative phenomena, where correlations between particles are so strong that standard independent particle approximations fail to give accurate predictions of system behavior. Unfortunately, even oversimplified models have proven extremely difficult to solve. This thesis will look at one of these models, the Ising model, in which spin one-half particles are fixed to lattice sites, and will investigate how the size of the lattice affects one of its properties, the Helmholtz free energy. This will be done by comparing numerical results for various size lattices with the predictions of graphical expansions.

A new Monte Carlo method which is based on the transfer matrix technique is developed to numerically solve this model. By sampling a random walk having the proper statistical features, estimates of the free energy, magnetization, and spin correlation are obtained.

A. The Ising Model

Consider a system of particles, with spin one-half, fixed at the vertices of a lattice. At each site, associate a binary scalar quantity, σ, which can be thought of as the projection of the spin. The spin can be thought of as pointing in some predefined direction in space (say, the +z direction) if $\sigma = +1$ and in the opposite direction if $\sigma = -1$.

Define the interaction energy between particles as follows:

(1.1) $E_{ij} = -a_{ij} J \sigma_i \sigma_j$; $a_{ij} = 1$ if spin i and spin j are nearest neighbors

$a_{ij} = 0$ otherwise

That is, if two nearest neighbors are pointed in the same direction, $E_{ij} = -J$; and if they are pointed in opposite directions $E_{ij} = +J$. Notice that J is a measure of the strength of the coupling, and $J > 0$ favors parallel spins by giving them a lower interaction energy.

Consider also that the system may interact with an external magnetic field. If each spin has a magnetic moment μ_s, its interaction with a field, $\vec{H} = H\hat{\ell}_z$, will be

(1.2) $$(E_H)_j = -\mu_s H \sigma_j$$

The full Hamiltonian for a lattice of N spins will be

(1.3) $$\mathcal{H}_I = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} J \sigma_i \sigma_j - \mu_s H \sum_{j=1}^{N} \sigma_j$$

or

(1.4) $$\mathcal{H}_I = -\sum_{<ij>} J \sigma_i \sigma_j - \mu_s H \sum_{j=1}^{N} \sigma_j$$

where $<ij>$ means sum over all nearest neighbor pairs.

Using the above Ising Hamiltonian, one can immediately write the canonical partition function

(1.5) $$Z = \sum\!\!\!\!\!\!- \exp[-\beta \mathcal{H}_I] \; ; \; \beta = \frac{1}{k_B T}$$

where the sum is over all system configurations, a configuration being a particular set of the values of all the spins. T is the absolute temperature; k_B is the Boltzmann constant. Equation (1.5) can also be expressed as:

(1.6) $$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \exp\left[\sum_{<ij>} K\sigma_i\sigma_j + h\sum_j \sigma_j\right]$$

(1.7) $$\text{where } K = \beta J \; ; \quad h = \beta \mu_s H$$

Notice that this problem can be reformulated in the language of quantum mechanics. Interpret the σ's as the Pauli matrices σ^z. To be precise

(1.8) $$\sigma_j = \underline{1} \times \underline{1} \times \ldots \sigma^z \ldots \times \underline{1} \times \underline{1}$$
$$\text{(1) (2) ... (j) ... (N-1) (N)}$$

(1.9) $$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} ; \quad \underline{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

where direct product notation has been used. That is, choose the direct product of all the spins of the lattice, with the σ^z's diagonal, as the representation. A general basis set will be written as

(1.10) $$|u\rangle = |\sigma_1, \sigma_2, \ldots \sigma_N\rangle ; \; \sigma's = \pm 1$$

and for a particular ket the following notation will be used

(1.11) $$|\uparrow\uparrow\downarrow\uparrow\ldots\rangle$$

The quantum Hamiltonian has the exact form as (1.5), since it is diagonal in this representation, but the σ's must be interpreted as operators. In this representation equation (1.5) becomes identically:

(1.12) $$Z = \mathrm{Tr}[e^{-\beta \mathcal{H}_I}]$$

The equilibrium thermodynamic variables follow in standard fashion. The free energy per spin:

(1.13) $$F = -\frac{k_B T}{N} \ell n\ Z \quad .$$

The internal energy per spin:

(1.14) $$U = -\frac{k_B T^2}{N} \frac{\partial(\ell n\ Z)}{\partial T}$$

and the magnetization per spin:

(1.15) $$\mathcal{M} \equiv \frac{\left\langle \sum_{j=1}^{N} \sigma_j \right\rangle}{N} = \frac{1}{N} \frac{\partial(\ell n\ Z)}{\partial h}$$

B. Physical Reality of the Model[1]

Mathematically, the problem is one of associating with each lattice site a binary variable, which for convenience has been taken as ±1. A Hamiltonian has been introduced which, as will be seen, favors ordered states.

This model can represent, in a simple way, the following three physical systems.

1. A magnetic system, where each binary variable represents the projection of the spin angular momentum of a particle fixed at the site.

(1.16) $$s^z = \frac{\sigma}{2}$$

At the time of the model's introduction, it was hoped that the Ising Hamiltonian would lead to an explanation of spontaneous magnetization, where all or most of the spins align. The language of spin systems was used in Section IA to introduce the model and will be used throughout this thesis.

2. A mixture of two kinds of molecules, say A and B. $\sigma = +1$ would mean that the site is occupied by an A atom, and $\sigma = -1$ would mean that the site is occupied by a B atom. This interpretation could lead to a description of ordering in binary alloys; for example, for $J > 0$, the Hamiltonian favors A atoms grouping with A atoms, and B atoms grouping with B atoms.

3. A mixture of atoms and holes, for which $\sigma = +1$ means that the site is occupied by an atom, and $\sigma = -1$ means that the site is vacant. Interpreted in this manner, the model is called a lattice gas, and could be used as a model for condensation.

The correspondence between the thermodynamic variables of the above three systems can be made rigorous. In particular, the isotherm $\mathcal{M}(h)$ for the magnetic problem can be easily transformed[2] into P(v), the pressure versus the specific volume for the lattice gas problem.

The approximate aspects of the model are the following:

1. fully localized spins (or atoms)
2. nearest neighbor interactions only
3. high anisotropy (spin system only).

However, cooperative phenomena are thought to be relatively independent of the explicit form of the Hamiltonian, especially at the critical point. Also, the Ising Hamiltonian must be understood before proceeding to more physical, and correspondingly, more difficult problems.

C. Order-Disorder Interpretation of the Model

To show how ordered states are preferred, let us look at the model from a statistical mechanical viewpoint. At zero field, the probability of the system being in the state

$$|u\rangle = |\sigma_1\sigma_2,\ldots\sigma_N\rangle \quad , \quad \sigma = \pm 1 \tag{1.17}$$

is

$$\Pr\{|u\rangle\} = Z^{-1}\left[e^{+J\sum_{\langle ij\rangle}\sigma_i\sigma_j/k_BT}\right] \tag{1.18}$$

At high temperatures, the denominator of the exponent dominates. All the states are nearly equiprobable, becoming so as $T \to \infty$. As the temperature is lowered, states which are highly ordered (i.e., large value of $J\sum_{\langle ij\rangle}\sigma_i\sigma_j$) have a higher probability than those that are less ordered. The lower the temperature, the greater the difference in the probability of two different states. Notice that this type of order does not prefer either the plus or minus z direction.

Upon adding a magnetic field, the probability becomes

$$\Pr\{|u\rangle\} = Z^{-1}\left[e^{+J\sum_{\langle ij\rangle}\sigma_i\sigma_j/k_BT}\right]\left[e^{+\mu H\sum_j\sigma_j/k_BT}\right] \tag{1.19}$$

The new factor $[e^{+\mu H\sum_j\sigma_j/k_BT}]$ breaks the symmetry, making more probable those states with spins pointing predominantly in the +z direction.

The above picture of a system becoming more ordered as the temperature is lowered does not, however, suggest either the presence or the absence of a phase transition.

D. A Brief History of the Model

In view of the voluminous literature on the Ising model, only the high points in its development will be covered. The

model was first formulated by Ernst Ising[4] in 1925. In his dissertation, suggested by his mentor Wilhelm Lenz, Ising exactly solved the model in one dimension, finding no phase transition.

The next important advance came in 1941 when Kramers and Wannier showed that the Ising partition function was the largest eigenvalue of a matrix, called the transfer matrix. By means of a symmetry argument, they found the critical point (K_c=.44069) of the 2D, $\infty \times \infty$, square lattice.

The above lattice with h = 0 was fully solved by Onsager[6] in 1942, who followed and extended the method of Kramers and Wannier. He obtained the same critical temperature, a continuous energy, and a specific heat that became infinite as $-\log|T-T_c|$, where T_c is the critical temperature.

A derivation of the spontaneous magnetization for the lattice was published in 1952 by C.N. Yang[7]. Griffiths[8], in 1968, showed that Yang's result is a lower bound to the true magnetization. An important set of inequalities was also developed by Griffiths[9]. One of them states that for the zero field case the covariance of any pair of spins is nonnegative (J>0); that is, the probability that they have the same sign is at least one-half. The above lattice in a finite magnetic field has yet to be exactly solved; in 3D nothing is known rigorously.

Many approximate methods have been used on the Ising model, in particular, the self-consistent field approach[10]. Since the cooperative phenomena are true many-body problems, these approximations did not reproduce the correct behavior of the thermodynamic variables. However, the use of exact series expansions

has proved extremely fruitful. A correspondence can be established between the exact power series expansion of the partition function and combinatorial problems in graph theory. For example, Wakefield[11] obtained the first twelve terms of the high temperature series for the zero field, simple cubic lattice. Knowledge of these terms has led to good approximations[12] of the thermodynamic variables.

II. Formulation of the Problem

A. Transfer Matrix Formalism

Basic to most problems in equilibrium statistical mechanics is the partition function Z, from which the free energy per particle (spin) can be obtained:

$$F = - \frac{k_B T}{N} \ell n \, Z \tag{2.1}$$

It will now be shown that the Ising partition function can be written as the largest eigenvalue of a matrix called the transfer matrix. Among the many proofs available, that of Kac[13] will be followed, for it is both the simplest and the most elegant.

First, the concept of layer must be defined. A lattice can be thought of as being composed of layers of sublattices. For example, in 1-D a single spin is a layer. For the 2-D square lattice, having n rows and m columns, a row of spins is a layer. Likewise, the 3-D simple cubic lattice of size $m \times n \times \ell$, has a 2-D square lattice ($m \times n$) as a layer.

There are two obvious, but important facts. First, the Ising Hamiltonian couples nearest neighbor layers. Second, knowing the configuration of all the layers uniquely fixes the configuration of the entire lattice.

The following derivation will be made explicitly using the square lattice. The argument extends trivially to the simple cubic lattice with only a redefinition of layer and changes in summation variables.

Denote the configuration of the jth layer, u_j. For example,

for the square lattice with n rows and m columns:,

$$(2.2) \qquad u_j = \{\sigma_1, \sigma_2, \ldots \sigma_m\} \; ; \qquad \sigma_\ell = \pm 1$$

the ordered set of all spin directions in the jth row. The partition function becomes

$$(2.3) \qquad Z = \sum_{\substack{\text{all system} \\ \text{configurations} \\ \text{(configs.)}}} \ell^{-\beta \mathcal{H}_I} = \sum_{\text{all layer 1 configs.}}$$

$$\sum_{\text{all layer 2 configs.}} \sum_{\text{all layer 3 configs.}} \cdots \sum_{\text{all layer n configs.}} \ell^{-\beta \mathcal{H}_I}$$

$$(2.4) \qquad Z = \sum_{u_1} \sum_{u_2} \cdots \sum_{u_n} + \ell^{-\beta \mathcal{H}_I}$$

Create periodic boundary conditions by wrapping the lattice on a cylinder so that the spins of the n'th row interact with the spins of the first row, and then bend the cylinder into a torus by having the spins of the first column interact with the spins of the last column. Then

$$(2.5) \qquad Z = \sum_{u_1, u_2, \ldots u_n} V_{u_1 u_2} V_{u_2 u_3} \cdots V_{u_n u_1}$$

where the 2^m dimensional matrix V is defined as:

$$(2.6) \quad \langle u|V|u' \rangle \equiv V_{uu'} \equiv \exp[K \sum_{j=1}^{m} \sigma_j \sigma_{j+1} + h \sum_{j=1}^{m} \sigma_j + K \sum_{j=1}^{m} \sigma_j \sigma_j']$$

where the first term in the exponential is the intralayer contribution, the second is the interlayer contribution, and the last contribution is from the field, where

$$\sigma_{m+1} = \sigma_1 \ , \tag{2.7}$$

and where a direct product basis of all the spins in a row is used:

$$\begin{aligned} |u\rangle &= |\sigma_1,\sigma_2,\sigma_3,\ldots\sigma_m\rangle \\ |u'\rangle &= |\sigma_1',\sigma_2',\sigma_3',\ldots\sigma_m'\rangle \qquad (2.8) \\ \sigma,\sigma' &= \pm 1 \ . \end{aligned}$$

Since all indices are dummy indices

$$Z = \sum_u (V_{uu})^n = Tr(V^n) = \sum_i \lambda_i^n \tag{2.9}$$

where the λ_i's are the eigenvalues of V

$$V|\Psi^i\rangle = \lambda_i|\Psi^i\rangle \ ; \quad \lambda_1 \geq \lambda_2 \geq \lambda_3\ldots \tag{2.10}$$

Now let the number of rows in the lattice become infinite.

$$Z = \sum_i \lambda_i^n = \lambda_1^n[1+ \sum_{i>1}(\frac{\lambda_i}{\lambda_1})^n] \tag{2.11}$$

$$\lim_{n\to\infty} (\frac{\ell n\ Z}{n}) = \ell n\lambda_1 \tag{2.12}$$

Furthermore, it can be shown[14] that the probability that the row j is in the state $|u_j\rangle$ is

$$\Pr\{|u_j\rangle\} = |\langle u_j|\Psi^1\rangle|^2 \tag{2.13}$$

B. Factorization of the Transfer Matrix

It has been shown that the partition function per row for an m by infinite lattice is the largest eigenvalue of the matrix V, the transfer matrix. V can be put into a more convenient form by factoring it into the product of simpler matrices[15]. Define the following 2^m dimensional matrices

$$(V_2)_{uu'} \equiv \delta_{uu'} \exp[K \sum_{j=1}^{m} \sigma_j \sigma_{j+1}] \tag{2.14}$$

$$(V_3)_{uu'} \equiv \delta_{uu'} \exp[h \sum_{j=1}^{m} \sigma_j] \tag{2.15}$$

$$(V_1)_{uu'} \equiv \exp[K \sum_{j=1}^{m} \sigma_j \sigma_j'] \tag{2.16}$$

consider

$$(V_2V_3V_1)_{uu'} = \sum_{u''u'''} (V_2)_{uu''}(V_3)_{u''u'''}(V_1)_{u'''u'} \tag{2.17}$$

$$= (V_2)_{uu}(V_3)_{uu}(V_1)_{uu'} \tag{2.18}$$

(2.19) $$= \exp[K \sum_{j=1}^{m} \sigma_j \sigma_{j+1} + h \sum_{j=1}^{m} \sigma_j + K \sum_{j=1}^{m} \sigma_j \sigma'_j]$$

(2.20) $$= V_{uu'}$$

Therefore

(2.21) $$V = V_2 V_3 V_1$$

V_1 can be put in the following form

(2.22) $$(V_1)_{uu'} = \exp[K \sum_{j} \sigma_j \sigma'_j] = \prod_{j} \exp[K \sigma_j \sigma'_j]$$

Looking at one factor in the (direct) product

(2.23) $$\exp[K \sigma_j \sigma'_j] = \begin{pmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{pmatrix}$$

(2.24) $$= \underline{1} e^{K} + \sigma^x e^{-K}$$

where

(2.25) $$\underline{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ; \quad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Therefore

(2.26) $$V_1 = \prod_{j} [e^{K} + \sigma_j^x e^{-K}]$$

where

$$\sigma_j^x = \overset{①}{1} \times \overset{②}{1} \times \ldots \overset{(j)}{\sigma^x} \ldots \times \overset{(m-1)}{1} \times \overset{(m)}{1} \tag{2.27}$$

Rewriting

$$V = V_2 V_3 V_1 \tag{2.21}$$

where

$$V_2 = \prod_j \exp[K\, \sigma_j \sigma_{j+1}] \tag{2.28}$$

$$V_3 = \prod_j \exp[h\sigma_j] \tag{2.29}$$

$$V_1 = \prod_j [e^K + \sigma_j^x e^{-K}] \tag{2.30}$$

Notice that

$$[V_2, V_3] = 0 \; ; \quad [V_2 V_1] \neq 0 \; ; \quad [V_3 V_1] \neq 0 \tag{2.31}$$

and that σ^x is a spin flipping operator

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \sigma^x \begin{pmatrix} 0 \\ 1 \end{pmatrix} ; \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \sigma^x \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.32}$$

C. The Character of the Largest Eigenvalue and Its Corresponding Eigenfunction

One general remark should be made about the 2^m dimensional transfer matrix. A theorem of Frobenius[16] states that for a finite dimensional matrix with all elements non-negative, the

largest eigenvalue is non-degenerate, and the corresponding ("largest") eigenvector has non-negative elements. For finite m, this theorem is obeyed by the transfer matrix, since all its elements are of exponential nature.

D. High Temperature Series Expansions

1. Introduction

High temperature series expansions for the Ising free energy will be derived for the bulk lattice and the finite lattice. It will be seen that the lowest order differences between them are the results of "surface" terms which contribute to the finite lattice, but not to the bulk lattice.

Following Fisher[17], the procedure for the expansion will be reviewed. On setting the magnetic field equal to zero, equation (1.12) becomes

$$Z = \mathrm{Tr}\left[\prod_{\langle ij\rangle} \exp(K\,\sigma_i\sigma_j)\right] \tag{2.33}$$

where the product is over all nearest neighbor bonds. Expanding the exponential in a power series, one sees that

$$\exp[K\,\sigma_i\sigma_j] = (\cosh K)(1+\sigma_i\sigma_j v) \;; \quad v = \tanh K \tag{2.34}$$

so that equation (2.33) becomes

$$Z = \cosh^{qN/2} K\ \mathrm{Tr}\left[\prod_{\langle ij\rangle} (1+\sigma_i\sigma_j v)\right] \tag{2.35}$$

where N is the number of spins; qN/2 is the number of bonds; q is four for the square lattice and six for the simple cubic lattice.

Now consider the expansion of the product. The coefficients of v^{ℓ} will be all combinations of all the different nearest neighbor bonds taken ℓ at a time.

However, for any i

$$\text{(2.36)} \qquad \mathrm{Tr}[(\sigma_i)^P] = \begin{cases} 0 & \text{when P is odd} \\ 2 & \text{when P is even.} \end{cases}$$

Therefore, all terms with an odd number of σ_i's will vanish under the trace. The surviving terms can be put in one-to-one correspondence with graphs drawn on the lattice. These graphs will be closed polygons since

a) from the nature of the expansion of the product, each bond can occur only once in each term

b) to survive the trace an even number of bonds must meet at any lattice point.

Therefore one can write

$$\text{(2.37)} \qquad Z = 2^N (\cosh^{qN/2} K)\left[1 + \sum_{\ell=0}^{\infty} P_\ell(N) v^\ell\right]$$

where $P_\ell(N)$ is the number of different graphs having ℓ bonds that can be drawn on a lattice of N sites.

2. The Bulk Lattice

The first few P_ℓ's of the square bulk lattice can be found by inspection.

(2.38) $$P_1(N) = P_2(N) = P_3(N) = 0$$

$$P_4(N) = N, \quad P_5(N) = 0, \quad P_6(N) = 2N \ .$$

Notice that $P_8(N)$ would have contributions both from octagons and separated squares.

By formally taking the logarithm, one can show that the series expansions for the free energy per spin become

(2.39) $$-\frac{F}{k_B T} = \ln 2 + \frac{q}{2} \ln \cosh K + \sum_{\ell=1}^{\infty} P_\ell^1 v^\ell$$

where P_ℓ^1 is the coefficient of the term in $P_\ell(N)$ which is linear in N. That is

(2.40) $$P_\ell(N) = NP_\ell^1 + N^2 P_\ell^2 + \ldots$$

This is to be expected from the intensive nature of the bulk free energy per spin.

3. The Finite Lattice

Consider a finite, periodic square lattice, of width m, wrapped on a cylinder of infinite length. All graphs of less than m bonds would contribute in the same way to both the finite and bulk lattices. However, when ℓ equals m, surface graphs[18] appear on the finite lattice but not on the bulk lattice. They are rings which circumscribe the cylinder, and they contribute

terms of order ν^m to the expansion of the partition function of the finite lattice. Higher order surface terms (of order ν^{m+2}, ν^{m+4} etc) can also be found.

Therefore, to leading order in ν

$$\frac{F_b}{k_B T} - \frac{F_f}{k_B T} = C(m)\nu^m \tag{2.41}$$

or

$$\frac{F_b}{k_B T} - \frac{F_f}{k_B T} = C(m)\exp[-m|\ell n\ \nu|] \tag{2.42}$$

where F_b is the free energy per spin of the bulk lattice, F_f is the free energy per spin of the finite lattice, and $C(m)$ is an unknown function of m.

Equation (2.42) shows, to lowest order, the size dependence of the free energy per spin.

To see this in more detail, contrast the expansion of the bulk lattice with the finite, $3 \times \infty$, periodic lattice.

$$Z_b(N) = 2^N \cosh^{qN/2} K[1+P_4(N)\nu^4+P_6(N)\nu^6+\ldots] \tag{2.43}$$

$$Z_f(N) = 2^N \cosh^{qN/2} K[1+S_3(N)\nu^3+P_4(N)\nu^4+S_5(N)\nu^5 + P_6(N)\nu^6+S_7(N)\nu^7+\ldots] \tag{2.44}$$

where $S_\ell(N)$ is the number of surface graphs having ℓ bonds that can be drawn on a lattice of N sites.

Therefore

$$(2.45)\quad -\frac{F_b}{k_B T} - \ell n\ 2 - \frac{q}{2}\ \ell n\ \cosh K = \frac{1}{N}[P_4\nu^4+P_6\nu^6+P_8\nu^8-\frac{P_4^2\nu^8}{2}+\ldots]$$

and

$$(2.46)\quad -\frac{F_f}{k_B T} - \ell n\ 2 - \frac{q}{2}\ \ell n\ \cosh K = \frac{1}{N}[S_3\nu^3+P_4\nu^4+S_5\nu^5+P_6\nu^6+S_7\nu^7 - \frac{S_3^2\nu^6}{2} - \frac{S_3P_4\nu^7}{2}+\ldots]$$

For this lattice then

$$(2.47)\qquad \frac{F_b}{k_B T} - \frac{F_f}{k_B T} = \frac{S_3\nu^3}{N} + O(\nu^5)$$

For the periodic simple cubic lattice of size $m \times m \times \infty$, the low order surface terms were found to be

$$(2.48)\qquad \frac{S_m(N)}{N} = 2/m\ ;\quad \frac{S_{m+2}(N)}{N} = 4(m-1)$$

$$(2.49)\qquad \frac{S_{m+4}(N)}{N} = 12(m-1) + \frac{4(m-1)(m-2)(m-3)}{3} + 12(m-1)(m-2)$$

III. The General Theory of Monte Carlo

As a formal definition of Monte Carlo, that of Shreider[19] will be used:

> The Monte Carlo method is a method of solving various problems in computational mathematics by constructing for each problem a random process with parameters equal to the required quantities of that problem. The unknowns are determined approximately by carrying out observations on the random process and by computing its statistical characteristics which are approximately equal to the required parameters.

A simple example, which has every feature of the above definition, is the integral

$$I = \int_a^b L(x)dx \tag{3.1}$$

Divide and multiply the integrand by:

$$\frac{P(x)}{c} \quad \text{where } P(x) > 0;\ c = \int_a^b P(x)dx \tag{3.2}$$

then

$$I = c\int_a^b \frac{L(x)}{P(x)}\left\{\frac{P(x)}{c}\right\} dx \tag{3.3}$$

If $\{P(x)/c\}$ is interpreted as a probability density, then

$$I = c\left\langle \frac{L(x)}{P(x)} \right\rangle \tag{3.4}$$

that is, the integral I is c times the average value of the function $\frac{L(x)}{P(x)}$, with respect to the density P(x)/c.

Suppose that one can obtain a sequence of numbers $x_1, x_2 \ldots x_N$, each sampled from the density P(x). Then[20] the following function, I_{EST}, is an unbiased stastistical estimate of the mean value of $C\frac{L(x)}{P(x)}$

$$(3.5) \qquad I \tilde{=} c \sum_{i=1}^{N} \frac{L(x_i)/P(x_i)}{N} \equiv I_{EST} \equiv c \left\langle \frac{L(x)}{P(x)} \right\rangle_{EST}$$

The samples x_1, $x_2 \ldots x_N$ need not be statistically independent. This particular form of estimator is called the sample mean.

Observe the trivial case where P(x) = L(x):

$$(3.6) \qquad I_{EST} = C \sum_{i=1}^{N} \frac{L(x_i)/L(x_i)}{N} = c \frac{N}{N} = c ,$$

making the estimator exact (zero variance). As suggested by the above trivial case, the statistical error δ

$$(3.7) \qquad \delta = |I - I_{EST}|$$

depends on the choice of P(x). Great increases in accuracy (efficiency) can be obtained by choosing P(x) such that the ratio $\frac{L(x)}{P(x)}$ remains as constant as possible over the range a,b. This procedure is called importance sampling. From the law of large numbers, the error also depends on N, the size of the sample. Other important theorems[21] (the central limit

theorem and the Chebyshev inequality) can be invoked to show that, when the samples are independent, the variance of the estimator is given by

$$(3.8) \qquad v(I_{EST}) \alpha \frac{1}{N} ,$$

and therefore the standard deviation of I_{EST}:

$$(3.9) \qquad S.D. = \sqrt{v}$$

$$S.D. \quad \alpha \frac{1}{\sqrt{N}}$$

By increasing the sample size, N, one can make the standard deviation as small as one likes. As one can estimate the mean value of a function, I, one can also estimate the standard deviation of I. In this thesis the estimated standard will be taken as the measure of error.

An estimator such as the sample mean, equation (3.5), is a random variable because it is a function of random numbers. It therefore has a density function associated with it. If, as is the situation with the sample mean, the mean of this new random variable equals the desired answer, the estimator is called an unbiased estimator. The difference between the mean of the above density function and the desired answer is called the bias.

IV. The Monte Carlo Method

A. The Relationship Between Random Walks and Eigenvalue Equations[22-23]

The largest eigenvalue of the transfer matrix and, therefore, the Ising partition function, will be obtained by simulating a random walk (a Markov chain with stationary transition probabilities) which has the proper statistical features. The walk will be conducted in a discrete space having the same dimensionality as the transfer matrix. A descriptive language will be used where points will be moved from one "position" in this space to another.

Consider the following eigenvalue equation with the operator A, the eigenvalue λ , and the eigenfunction $|\phi\rangle$

$$|\phi\rangle = \frac{A}{\lambda}|\phi\rangle \tag{4.1}$$

In a discrete space A is a matrix; in a continuous space A is an integral operator. In what follows, the notation of the discrete case will be used.

Consider first the special case where the operator $(\frac{A}{\lambda})$ is stochastic; that is,

$$\frac{Auu'}{\lambda} \geq 0, \text{ all } u,u' \; ; \quad \sum_{u}(\frac{Auu'}{\lambda}) = 1, \text{ all } u' \; . \tag{4.2}$$

(Notice that the discrete space is labeled using the same indices as the direct product spin space used for the transfer matrix.)

Equation (4.1) may now be given a probabilistic interpretation. Let $|\phi\rangle$, the eigenfunction, be a probability density function:

$$\Pr\{u\} = \langle u|\phi\rangle = \phi_u \ . \tag{4.3}$$

That is, the probability of the point being at position u is ϕ_u. Because equation (4.1) is linear and homogeneous, the probability can be taken as normalized:

$$\sum_u \langle u|\phi\rangle = 1 \ . \tag{4.4}$$

Also, let $(\frac{A}{\lambda})_{uu'}$ be the conditional probability of u, given u':

$$\Pr\{u|u'\} = \langle u| \frac{A}{\lambda} |u'\rangle = (\frac{A}{\lambda})_{uu'} \ . \tag{4.5}$$

That is, the probability of the point moving to u, given that it is at u', is $(\frac{A}{\lambda})_{uu'}$. Notice that equation (4.4) gives the required normalization. Equation (4.1) can be written as

$$\phi_u = \sum_{u'} (\frac{A}{\lambda})uu'\phi_{u'} \tag{4.6}$$

and interpreted as follows:

> The probability of being at u after the move, ϕ_u, equals the probability of being at u' before the move, $\phi_{u'}$, times the probability of moving to u from u', $(\frac{A}{\lambda})_{uu'}$, summed over all u'.

ϕ is therefore the stable, steady state density for a point, or

a population of points which moves by means of the "kernel", $\frac{A}{\lambda}$.

This process can easily be simulated. Given a population of points, with positions u', distributed according to $\phi_{u'}$, move each of them independently to a new position, u, by sampling $(\frac{A}{\lambda})_{uu'}$. The process of all points in the population making a move will define one iteration. By equation (4.6), the population after the iteration will still be distributed according to ϕ. However, since both ϕ and λ are not known, a procedure of convergence must be found. More about this important consideration will follow.

The eigenvalue equation can be generalized to

$$(4.7) \qquad |\phi\rangle = \frac{BA}{\lambda}|\phi\rangle \ ,$$

where

A is stochastic, $\sum_u A_{uu'} = 1$; $A_{uu'} \geq 0$ all u,u'

B is positive and diagonal, $B_{uu'} = \delta_{uu'}B_u$; $B_{uu'} \geq 0$ all u,u'

and λ is the eigenvalue of the operator BA.

Rewriting

$$(4.8) \qquad \phi_u = \sum_{u'} \frac{B_u}{\lambda} A_{uu'} \phi_{u'} \ .$$

The new matrix, $\frac{B}{\lambda}$, can be incorporated into the above scheme by introducing the following fissioning technique. Create an arbitrary set of probability density functions $g_u(\xi)$ on the space

of non-negative integers ξ such that

$$(4.9) \qquad \langle \xi \rangle_{g_u(\xi)} = B_u/\lambda \equiv F_u \ .$$

This mean value will be called the fissioning part of the matrix. Use them in the following way. When a point moves from u' to u, sample $g_u(\xi)$ for a ξ . Fission the point such that it becomes ξ points at u. Then move all these "daughters" independently. For a proof that this procedure will simulate equation (4.7), see Appendix A.

One last generalization of the eigenvalue equation is needed. Consider:

$$(4.10) \qquad |\phi\rangle = \frac{BA}{\lambda}|\phi\rangle \ ,$$

where now,

B is still diagonal and positive

A is positive (not necessarily stochastic).

Rewriting,

$$(4.11) \qquad \phi_u = \sum_{u'} \frac{B_u A_{uu'}}{\lambda} \phi_{u'} \ .$$

Choose an arbitrary conditional probability, $P_{uu'}$, whose norm is known:

$$(4.12) \qquad P_{uu'} > 0 \text{ all } u,u' \ ; \qquad \sum_{u} P_{uu'} = C_{u'} \ ;$$

that is,

$$\Pr\{u|u'\} = P_{uu'}/C_{u'} \quad . \tag{4.13}$$

Multiply and divide equation (4.11) by this conditional probability

$$\phi_u = \sum_{u'} \frac{B_u C_{u'}}{\lambda} \frac{A_{uu'}}{P_{uu'}} \left\{ \frac{P_{uu'}}{C_{u'}} \right\} \phi_{u'} . \tag{4.14}$$

Now consider the random walk which arises from this equation. Move the points from u' to u by sampling $\frac{P_{uu'}}{C_{u'}}$.

Upon arrival of a point at u, fission the point to ξ daughters such that

$$\langle \xi \rangle = \frac{B_u C_{u'}}{\lambda} \frac{A_{uu'}}{P_{uu'}} \equiv F_{uu'} \quad . \tag{4.15}$$

The right-hand side of this equation will again be called the fissioning part of the matrix.

Because of the freedom one has in choosing $P_{uu'}$, many different random walks have the same density $|\phi\rangle$. This is just importance sampling (see Chapter III) applied to linear equations, and, here also, great increases in accuracy and stability can be had by choosing $P_{uu'}$ such that the fissioning part of the matrix,

$$\frac{B_u C_{u'}}{\lambda} \frac{A_{uu'}}{P_{uu'}} \quad , \tag{4.16}$$

remains as constant as possible.

B. Convergence

The relationship between stable random walks and eigenvalue problems was established in the previous section. Since neither the eigenfunction nor the eigenvalue is known, a method is needed to provide convergence (relaxation) from a trial eigenfunction to the true eigenfunction. Let $\vec{\phi}_\ell$ be the vector particle density after the ℓ'th iteration. $\vec{\phi}_0$ then is the trial eigenfunction, here regarded as a density function. Also, let λ_T be the trial eigenvalue. Consider the following game:

1. Sample a population of points from $\vec{\phi}_\ell$; $\ell = 0$.
2. Move and fission each point in the population independently, as described in the previous section. From the discussion following equation (4.6), it can be seen that

$$\vec{\phi}_{\ell+1} = \frac{BA}{\lambda} \vec{\phi}_\ell \quad . \tag{4.17}$$

   That is, if the population was distributed according to $\vec{\phi}_\ell$ before the move, it is distributed according to $\vec{\phi}_{\ell+1}$ after the move.
3. $\ell \Rightarrow \ell + 1$; go to step 2 until $\ell \geq \ell_{MAX}$; then go to step 4.
4. Stop.

Looking at the analytic features of the game, let ϕ^i and λ_i be the eigenvectors and eigenvalues of BA ordered such that

(4.18) $$\lambda_1 > \lambda_2 > \lambda_3 \cdots .$$

Expand ϕ_o in eigenfunctions of BA:

(4.19) $$\vec{\phi}_o = \sum_i C_i \vec{\phi}^i \quad , \qquad C_i = \langle \phi^i | \phi_o \rangle \ .$$

Then, from equation (4.17),

(4.20) $$\vec{\phi}_1 = \sum_i C_i \left(\frac{\lambda_i}{\lambda_T}\right) \vec{\phi}^i$$

and

(4.21) $$\vec{\phi}_\ell = \sum_i C_i \left(\frac{\lambda_i}{\lambda_T}\right)^\ell \vec{\phi}^i \ .$$

Let $\lambda_T = \lambda_i$. Then,

(4.22) $$\vec{\phi}_\ell = C_1 \vec{\phi}^1 + \sum_{i=2} \left(\frac{\lambda_i}{\lambda_1}\right)^\ell C_i \vec{\phi}^i$$

Assuming no degeneracy,

(4.23) $$\lim_{\ell \to \infty} \vec{\phi}_\ell = C_1 \vec{\phi}^1 \ .$$

Therefore, for large ℓ (after relaxation), the above game produces a poplulation of points drawn from ϕ^1, the "largest" eigenfunction of BA.

The speed of convergence can be seen to depend on:

1. The size of C_1, i.e. how good the trial eigenvector is.
2. The ratio of λ_2 to λ_1.

Those readers familiar with standard numerical methods can see that the above method is the stochastic analog of the Neuman iteration method.

Essential to the above proof are the conditions

$$\langle u|\phi^1\rangle \geq 0 , \quad \text{all } |u\rangle , \tag{4.24}$$

as these numbers are interpreted as probabilities. The "largest" eigenfunction of the transfer matrix has been shown in Section II.C to satisfy these conditions.

C. Applying Monte Carlo to the Transfer Matrix

The concepts of Section IV. A will be applied to the eigenvalue equation

$$|\Psi\rangle = \frac{V}{\lambda}|\Psi\rangle , \tag{2.10}$$

where V is the transfer matrix and λ is its largest eigenvalue. By suitably factoring, V may be put in the form of BA (equation (4.7) or (4.10)). The discrete space in question is the direct product spin space of all the spins in a layer (row, for 2-D). Points then will move from layer configuration $|u'\rangle$ to layer configuration $|u\rangle$. This is conceptually equivalent to having spins in $|u'\rangle$ flip so that the configuration becomes $|u\rangle$. From the explicit form of the transfer matrix it will be seen that this is indeed what happens.

1. The Obvious Walk

It has been seen in Section IV. A that different random walks have the same density $|\phi\rangle$. Also, the method of creating and simulating them was shown. Because of the previous splitting of V into three matrices, $V_2V_3V_1$, V_2V_3 being diagonal, an obvious random walk can be constructed using V_1 as the moving factor and V_2V_3 as the fissioning factor. Because of its pedagogical value, and because it was the first walk computed for this thesis, it will be examined in detail.

The transfer matrix for a 2-D square lattice with m spins per row is

$$V = V_2V_3V_1 \ , \tag{2.21}$$

where

$$V_2 = \prod_j \exp(K\sigma_j\sigma_{j+1}) \ , \tag{2.28}$$

$$V_3 = \prod_j \exp(h\sigma_j) \ , \tag{2.29}$$

and

$$V_1 = \prod_j [e^K + \sigma_j^x e^{-K}] \ . \tag{2.30}$$

After dividing and multiplying V_1 by $\prod(e^K+e^{-K})$ and defining

$$P \equiv (e^{2K}+1)^{-1} \quad , \quad 0 \leq P \leq 1 \ , \tag{4.25}$$

V_1 takes the form

$$V_1 = (2 \cosh k)^m \prod_{j=1}^{m} [(1-P)+\sigma_j^x P] \quad . \tag{4.26}$$

Now remove the number $(2 \cosh k)^m$ from V_1 and place it with V_2 so that new operators are defined as

$$\left\{ \begin{array}{l} \tilde{V}_2 = (2 \cosh k)^m \prod_j \exp(K\sigma_j\sigma_{j+1}) \\ \tilde{V}_1 = \prod_{j=1}^{m} [(1-P)+\sigma_j^x P] \\ V = \tilde{V}_2 V_3 \tilde{V}_1 \end{array} \right\} \tag{4.27}$$

Since $\tilde{V}_2 V_3$ is diagonal, it has the properties of the B matrix of the second walk in Section IV. A:

$$\tilde{V}_2 V_3 \Leftrightarrow B \quad . \tag{4.28}$$

Now the matrix $\tilde{V}_1$ must be checked to see if it is stochastic; if so, it corresponds to the matrix A of the previous section. V_1 is stochastic if

$$\sum_u \langle u|\tilde{V}_1|u'\rangle = 1 \quad \text{for any } |u'\rangle \quad . \tag{4.29}$$

Consider the expansion of the product

$$\tilde{V}_1 = \prod_{j=1}^{m} [(1-P)+\sigma_j^x P] \quad . \tag{4.30}$$

Remembering that σ^x is a flip flop operator, that the $|u\rangle$'s are orthogonal, and using combinatorial theory, the coefficient, a, of the $|u\rangle$ 'th component of $\tilde{V}_1|u'\rangle$ is

$$a = (1-P)^{m-NFD} P^{NFD} , \tag{4.31}$$

where NFD is the number of spin flips necessary to change u' into u. Therefore,

$$\langle u|\tilde{V}_1|u'\rangle = (1-P)^{m-NFD} P^{NFD} . \tag{4.32}$$

Now the number of kets which differ from $|u'\rangle$ by NFD spins is just the binomial coefficient

$$\binom{m}{NFD} = \frac{m!}{NFD!(m-NFD)!} \tag{4.33}$$

Hence,

$$\sum_u \langle u|\tilde{V}_1|u'\rangle = \sum_{NFD=0}^{m} \binom{m}{NFD} (1-P)^{m-NFD} P^{NFD} = [(1-P)+P]^m = 1 \tag{4.34}$$

using the binomial theorem. Consequently, V_1 is stochastic, so that

$$\tilde{V}_1 \Leftrightarrow A \qquad \text{(stochastic case)} . \tag{4.35}$$

One important question remains. How does one move a particle according to the conditional probability $(\tilde{V}_1)_{uu'}$; that is, given a particle is at u', how does one sample $(\tilde{V}_1)_{uu'}$ for a new position u? The following routine will do the job:

> Independently, and with probability P, flip each of the m spins in $|u'\rangle$ $(=|\sigma_1', \sigma_2' \ldots \sigma_m'\rangle)$. The resulting ket $|u\rangle$ is drawn from $(\tilde{V}_1)_{uu'}$.

The proof is simple. From equation (4.32),

$$(\tilde{V}_1)_{uu'} = P^{NFD}(1-P)^{m-NFD} \quad , \tag{4.36}$$

but the right-hand side of equation (4.36) is just the probability of moving from $|u'\rangle$ to $|u\rangle$ by the above routine.

2. An Improved Walk

The walk outlined in the previous section proved unsatisfactory. Lattices no larger than $4 \times 4 \times \infty$ (three dimensions) could be simulated because of the poor stability and accuracy of the walk. The major reasons for this can be seen. The fact that each spin in $|u'\rangle$ was flipped independently means that most of its correlation with both other spins and the magnetic field was supplied by the fissioning factor $\frac{B_u}{\lambda}$, after the move was completed. Therefore, if a particle happened to move to a part of space with a large value of $\sum \sigma_i \sigma_{i+1}$ and $\sum \sigma_i$, it produced many daughters. Conversely, if it moved to an unproductive part of space, it produced no daughters. From

the point of view of importance sampling, this is just what should be avoided.

By use of importance sampling, the following improved walk was devised. Given the ket

$$u' = |\sigma_1', \sigma_2', \ldots \sigma_m'\rangle \tag{4.37}$$

build the ket

$$u = |\sigma_1 \sigma_2 \ldots \sigma_m\rangle \tag{4.38}$$

in the following way:

1. Flip the first spin such that $\langle \sigma_1 \rangle = M$, where M is a guess of the system magnetization.
2. Flip the next spin, to the value σ_i, conditional on σ_i' and the result σ_{i-1}, in a manner to be explained.
3. Repeat step 2 for all but the last spin.
4. Flip the last spin to the value σ_M conditional on σ_M, and the results σ_{M-1} and σ_1.

It can be seen that this procedure can build into the jump not only a preference for the spins to align with the magnetic field, but also a preference to align with themselves. We now investigate this in detail. Given

$$\langle u|V|u'\rangle = \langle u|V_2 V_3 V_1|u'\rangle \tag{4.39}$$

$$= (V_2)_u (V_3)_u (V_1)_{uu'} ,$$

being careful to obey the commutation relations and explicitly using periodic boundary conditions, define the following "single" spin operators

$$(4.40)\qquad \langle u|V|u'\rangle = (V_2)_{\sigma_1}(V_2V_3)_{\sigma_m}(V_1)_{\sigma_m\sigma'_m}\ldots(V_2V_3)_{\sigma_2}(V_1)_{\sigma_2\sigma'_2}(V_3)_{\sigma_1}(V_1)_{\sigma_1\sigma'_1}$$

where

$$(4.41)\qquad (V_1)_{\sigma_i\sigma'_i} = \langle\sigma_i|e^{-K_+e^K\sigma^x}|\sigma'_i\rangle ,$$

$$(4.42)\qquad (V_3)_{\sigma_i} = \exp[h\sigma_i] , \qquad (V_2(\sigma_{i-1}))_{\sigma_i} = \exp[K\sigma_i\sigma_{i-1}] ,$$

$$(4.43)\qquad \sigma_0 = \sigma_M .$$

For step one above, multiply and divide the matrix element by $P_{\sigma_1\sigma'_1}$, defined such that

$$(4.44)\qquad \langle\sigma_1\rangle_{P_{\sigma_1\sigma'_1}} = M ;$$

that is,

$$(4.45)\qquad \ldots(V_2V_3)_{\sigma_2}(V_1)_{\sigma_2\sigma'_2}(V_3)_{\sigma_1}\frac{(V_1)_{\sigma_1\sigma'_1}}{P_{\sigma_1\sigma'_1}}\left\{P_{\sigma_1\sigma'_1}\right\}.$$

For step 2 do the following: Define the (unnormalized) probability.

$$(4.46) \qquad \Pr\{\sigma_2|\sigma_2',\sigma_1\} \equiv (V_2(\sigma_1)V_3)_{\sigma_2}(V_1)_{\sigma_2\sigma_2'};$$

$C(\sigma_2',\sigma_1)$ is its normalization:

$$(4.47) \qquad C(\sigma_2',\sigma_1) = \sum_{\sigma_2} (V_2V_3)_{\sigma_2}(V_1)_{\sigma_2\sigma_2'} \quad .$$

Again divide and multiply the matrix element:

$$(4.48)\ldots \frac{C(\sigma_2',\sigma_1)(V_2V_3)_{\sigma_2}(V_1)_{\sigma_2\sigma_2'}}{\Pr\{\sigma_2|\sigma_2',\sigma_1\}} \left\{ \frac{\Pr\{\sigma_2|\sigma_2'\sigma_1\}}{C(\sigma_2',\sigma_1)} \right\} \frac{(V_1)_{\sigma_1\sigma_1'}}{P_{\sigma_1\sigma_1'}} \left\{ P_{\sigma_1\sigma_1'} \right\} .$$

On simplifying this becomes:

$$(4.49) \quad \langle u|V|u' \rangle = \ldots C(\sigma_2'\sigma_1) \left\{ \frac{\Pr\{\sigma_2|\sigma_2'\sigma_1\}}{C(\sigma_2'\sigma_1)} \right\} \frac{(V_1)_{\sigma_1\sigma_1'}}{P_{\sigma_1\sigma_1}} \left\{ P_{\sigma_1\sigma_1} \right\},$$

where the two terms in curly brackets become the flipping probabilities, and the other two terms become the developing fission factor.

Step 3 can be seen to be a generalization of step 2, in which the flipping probability for the m'th spin becomes conditional on σ_m',σ_{m-1}, and σ_1.

By use of this revised scheme, the efficiency of the computation was increased by a factor of magnitude 10^3 relative to the first walk, and was used in the final calculations.

D. Estimating the Eigenvalue and Its Logarithm

The random walk as described in the previous sections will provide a population of points whose distribution is Ψ, the "largest" eigenvector of the transfer matrix. What is desired is the largest eigenvalue, λ, which is the partition function per layer, and the free energy per spin, $F(N^*)$:

$$F(N^*) = - \frac{k_B T}{N^*} \ell n \, \lambda , \tag{4.50}$$

where N^* is the number of spins per layer.

In the previous sections, it had been assumed that λ was known. This not being the case, suppose a trial eigenvalue, λ_T, is used. In Appendix A it is shown that the mean number of daughters per point is unity if $\lambda_T = \lambda$. Since $\frac{1}{\lambda_T}$ is a constant multiplying $V|\Psi\rangle$, this statement may be generalized to

$$\left\langle \frac{\text{\# of daughters}}{\text{points}} \right\rangle = \lambda/\lambda_T , \tag{4.51}$$

or

$$\lambda = \lambda_T D ; \qquad D \equiv \left\langle \frac{\text{\# daughters}}{\text{point}} \right\rangle \tag{4.52}$$

Therefore a Monte Carlo estimator of λ is:

$$\lambda_{EST} = \lambda_T \, D_{EST} \tag{4.53}$$

where D_{EST}, the estimator for the mean number of daughters per

point, can be scored in the following manner. Let P_i be the number of points in the i'th iteration. Assume that the i'th to the (i+m)'th iterations are to be scored; then an estimator is the sample mean

$$D_{EST} = \frac{\sum_{K=i+1}^{i+m} P_K}{\sum_{K'=i}^{i+m-1} P_{K'}} \tag{4.54}$$

If the population is distributed according to Ψ, i.e., fully converged, this estimator is unbiased. However, a better estimator (lower variance) would be:

$$\lambda_{EST} = \lambda_T \sum_{i=1}^{Q} (F_{uu'})_i / Q \ , \tag{4.55}$$

where Q is the total number of points that moved in the above block of iterations (see discussion concerning equation (4.15)). This was the estimator used.

Perform the above procedure for several different blocks of iterations, obtaining several different estimates, and form their sample mean, M_{EST}. The result, i.e., the random variable, M_{EST}, with mean D and unknown variance, will, by the central limit theorem, be assumed to have a normal distribution.

To obtain the free energy, equation (4.50), an estimate of $\ell n\ \lambda_1$ is needed. Now, the mean of the random variable, $\ell n\ M_{EST}$, is not equal to ℓn D, but as shown in Appendix B, the effect of the bias can be neglected.

Therefore, the following estimator for the free energy was used:

$$\frac{-F_{EST}(N^*)}{k_B T} = \frac{1}{N^*} [\ell n\ \lambda_T + \ell n\ M_{EST}] \ . \tag{4.56}$$

V. A Technical Description of the Programs

Because the programs for the two-and three-dimensional Ising models differ only in the meaning of a layer and the geometry of the interactions, only the program for the two-dimensional model will be described.

Working in a direct product (σ^z) representation of dimensionality 2^m, basis kets (row configurations) were represented by computer words, each of the first m bits of a word representing the value (±1) of its respective spin. For example, for a five-spin-per-row lattice, a possible basis ket would be

(5.1) $$|\uparrow\downarrow\uparrow\downarrow\downarrow\rangle \quad ,$$

and would be represented by the computer word

(5.2) $$\text{KET} = 10100\ldots$$

Since a sixty-bit computer was used, any value of m less than sixty one could be accommodated without further bookkeeping.

Routines were created for the following purposes:

1. To create a random ket from a given distribution.
2. To flip, with known probability, the j'th spin in a given ket($0<j\leq m$).
3. To find the number of up spins ($\sigma_j=+1$) in a given ket.
4. To find the number of positive bonds ($\sigma_j\sigma_{j+1}=+1$) in a given ket.

5. To sense the direction of the j'th spin.

To create an initial population sampled from ϕ_o, the positions (u) of approximately two thousand points were drawn from a distribution in u space, in which each spin component had the same independent probability of being up; that is

$$(\phi_o)_u = p(\sigma_1)p(\sigma_2)\ldots p(\sigma_m) , \quad \sigma_j = \pm 1 \tag{5.3}$$

where

$$p(\sigma_j=+1) = 1 - p(\sigma_j=-1) , \quad \text{all } j . \tag{5.4}$$

By equation (2.13), p should be chosen close to unity for a region of temperature and field in which the magnetization per spin is expected to be close to one, and should be chosen close to one half in a region in which the magnetization per spin is expected to be close to zero.

As described in Section IV. A, each point in the population was then independently moved from its position $|u'\rangle$ to its new position $|u\rangle$ by flipping, with known probability, each spin in the ket $|u'\rangle$. The point was then split into ξ points by sampling a ξ from $g_{uu'}(\xi)$. This was done in the following manner. Suppose that when the point was moved from $|u'\rangle$ to $|u\rangle$, the numerical value of the fissioning part of the matrix was $F_{uu'}$. Let I be the integral part and F_r be the fractional part of $F_{uu'}$; i.e.,

(5.5) $$F_{uu'} = I + F_r \ ;$$

with probability F_r let $\xi = I + 1$;

with probability $1 - F_r$ let $\xi = I$.

Then ξ is a random variable with mean

(5.6) $$\langle \xi \rangle = F_r(I+1) + (1-F_r)I = I + F_r = F_{uu'} \ .$$

Therefore ξ satisfies equation (4.15).

Successive Monte Carlo iterations were performed until stability was reached. During this convergence, the trial eigenvalue was adjusted in the following way:

(5.7) $$\lambda_T = \frac{N_A}{N_B} \lambda_T \ ,$$

where N_A is the number of points after the move and N_B the number before the move. Convergence to Ψ was assumed completed after it was noticed that λ_T had small fluctuations about a relatively stable value. Arrival at Ψ was further spot checked by performing a very long chain of iterations, thereby watching the long term behavior of λ_T.

After convergence was completed, λ_T was held fixed and the iterations were continued. Equation (4.56) was used as a Monte Carlo estimator of the free energy.

To check the Monte Carlo results, a numerical procedure was developed for solving the square, three-spin-per-row problem

(m=3) . The resulting eight-by-eight transfer matrix was diagonalized by standard numerical methods. Both above and below the critical temperature the Monte Carlo result agreed with the numerical result to within a few parts in ten thousand. Also, the error was always the same order of magnitude as the estimated standard deviation.

VI. Results

Using the previously described Monte Carlo procedure, the zero-field free energy was found for simple cubic lattices of various sizes. Also, the exact series expansion (to v^{12}) of Wakefield was summed at the same temperature to give a good approximation of the bulk free energy. The "temperature" chosen was $K_c/1.83$, high enough that the series in $v(\tanh K=.17)$ was rapidly converging. Table 1 contains the numerical results, wherin the interval of error is twice the estimated standard deviation. A plot of free energy versus lattice size is shown in Figure 1. The effect of surface terms (equations 2.48 and 2.49) can be seen by subtracting them from the Monte Carlo results (Fig.2).

As explained in Appendix C, the magnetization and spin correlation were also obtained. Figure 3 shows a sample magnetic isotherm at "temperature" $K_c/1.25$, slightly above the critical point. The corresponding numerical data are contained in Table 3.

Defining $\rho(r)$ as the spin correlation at zero field

$$\rho(r) = \langle \sigma_i \sigma_{i+r} \rangle , \tag{6.1}$$

in which both spins are in the same row, both the nearest neighbor, r = 1, and the next-nearest neighbor, r = 2, spin correlations are shown in Figure 4 for various temperatures down to the critical point. Table 4 contains the corresponding numerical results. A plot of $\rho^2(1)$ versus $\rho(2)$ is shown in Figure 5.

TABLE 1

Free energies of the simple cubic lattice

N^*	$-F(N^*)/k_BT$	$-F_r(N^*)/k_BT$	$-F_b/k_BT$
9	$.717270 \pm 1.9\times10^{-5}$	.715880	.7158219049
16	$.715951 \pm 1.1\times10^{-5}$	.715804	
25	$.715864 \pm 4.7\times10^{-6}$	.715847	
49	$.715828 \pm 5.4\times10^{-6}$	.715828	
121	$.715822 \pm 6.3\times10^{-6}$	.715822	

$F(N^*)$ is the free energy per spin for a lattice with N^* spins per layer.

$F_r(N^*)$ is the same free energy with all surface terms, to order $m + 4$, removed.

F_b is the bulk free energy.

TABLE 2

Magnetization per spin for cubic lattice with 121 spins per layer

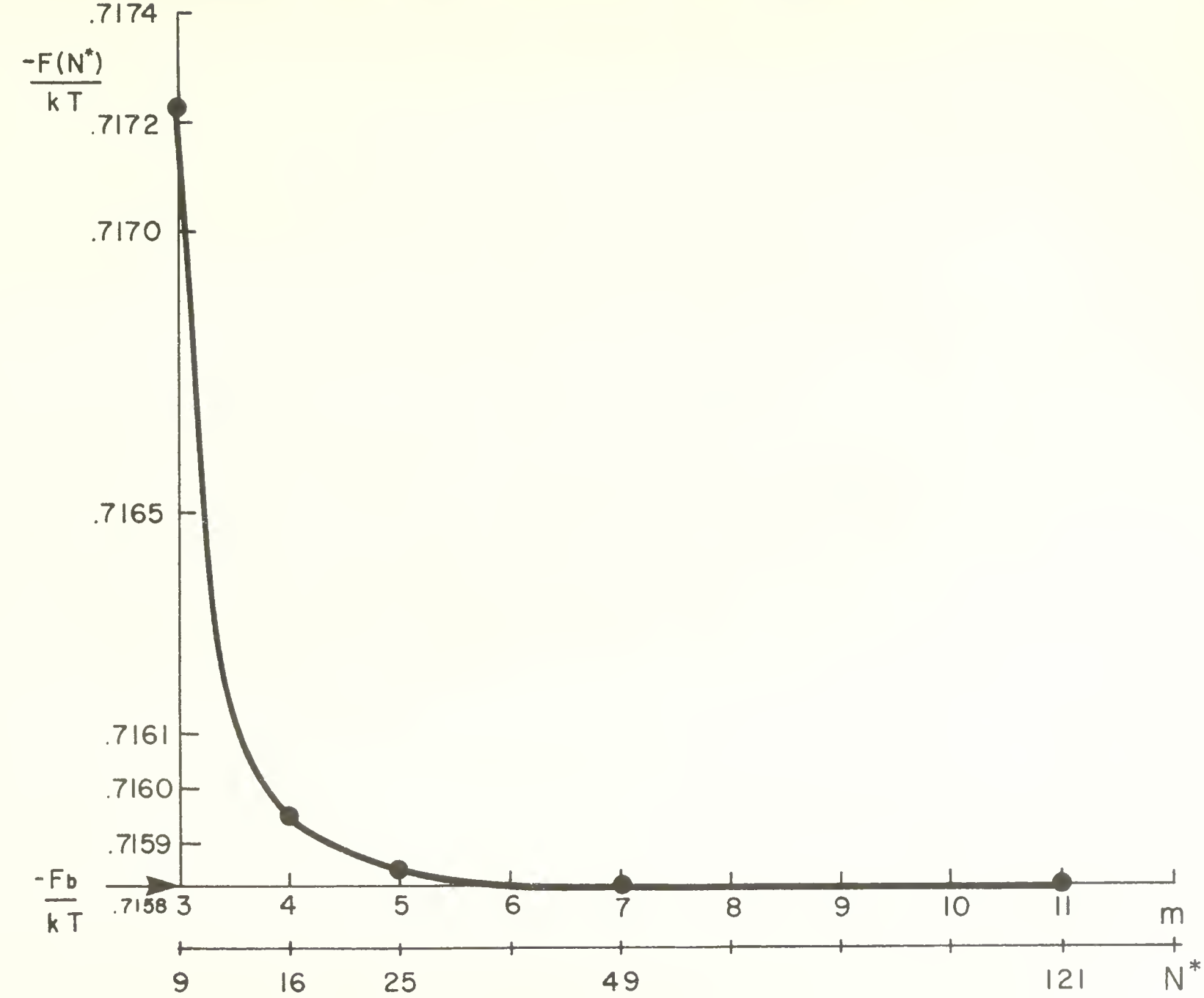
tanh(h)	M(h)
.025	.1955 ± .005
.05	.3295 ± .01
.1	.4898 ± .015
.2	.6456 ± .004
.4	.8156 ± .007
	$K = K_C/1.25 = .17737$

TABLE 3

Spin correlation for a cubic lattice with 121 spins per layer

K	ρ(1)	ρ(2)
$K_C/1.83 = .12115$	.12979 ± .00098	.01597 ± .0010
$K_C/1.50 = .14781$	.16284 ± .0012	.02896 ± .0015
$K_C/1.25 = .17737$	.20676 ± .0031	.05384 ± .0027
$K_C = .22171$	.30557 ± .011	.12830 ± .017

figure 1 Free energy versus lattice size



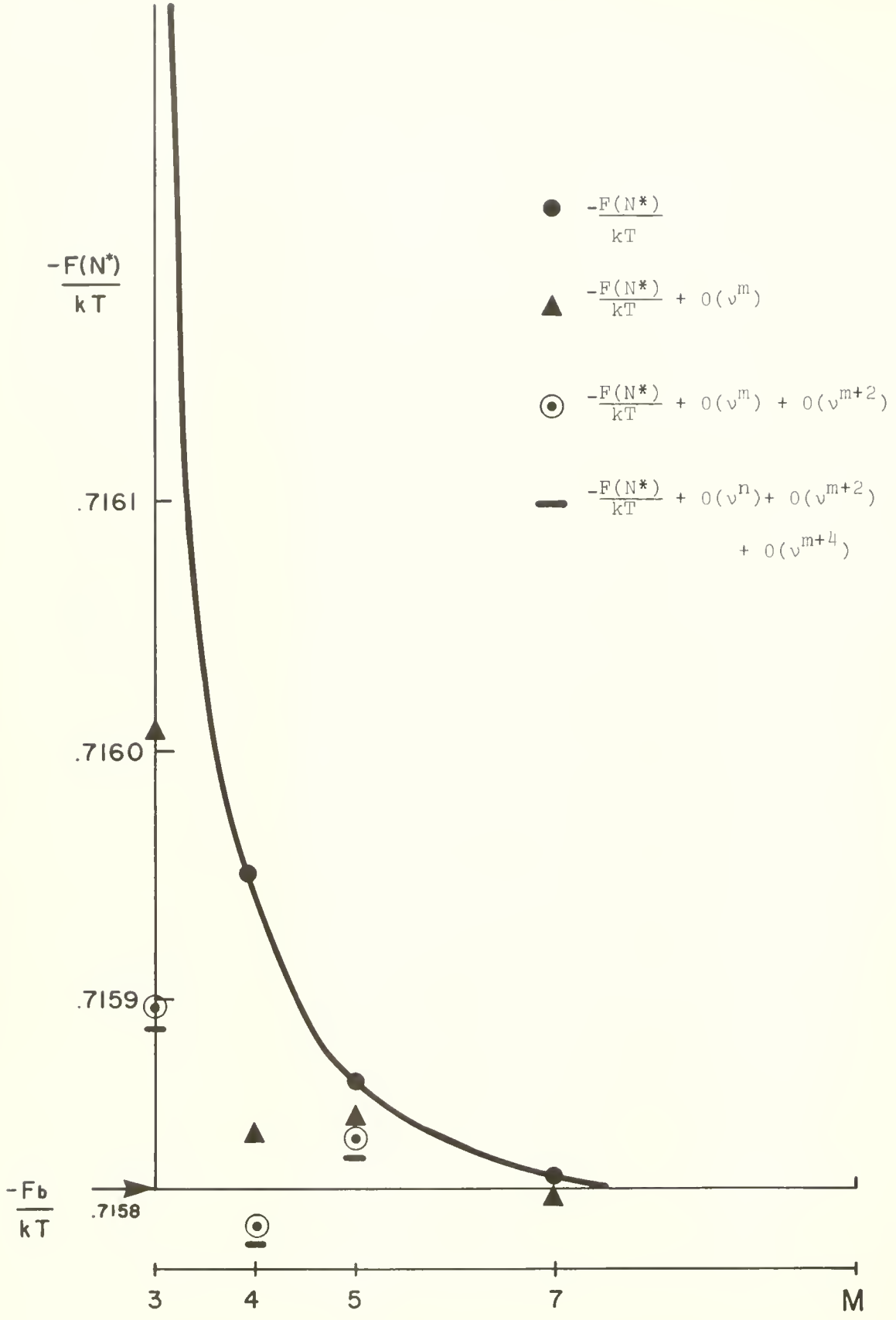


figure 2 The effect of surface terms

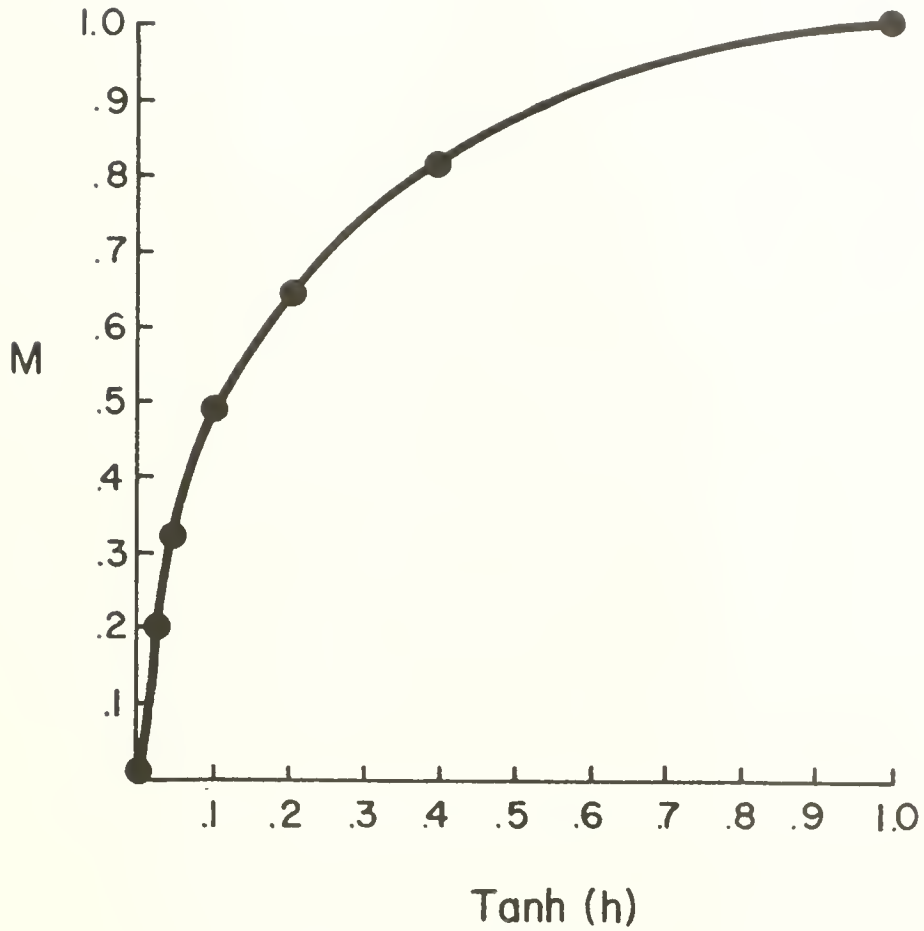


figure 3 Magnetization Per Spin

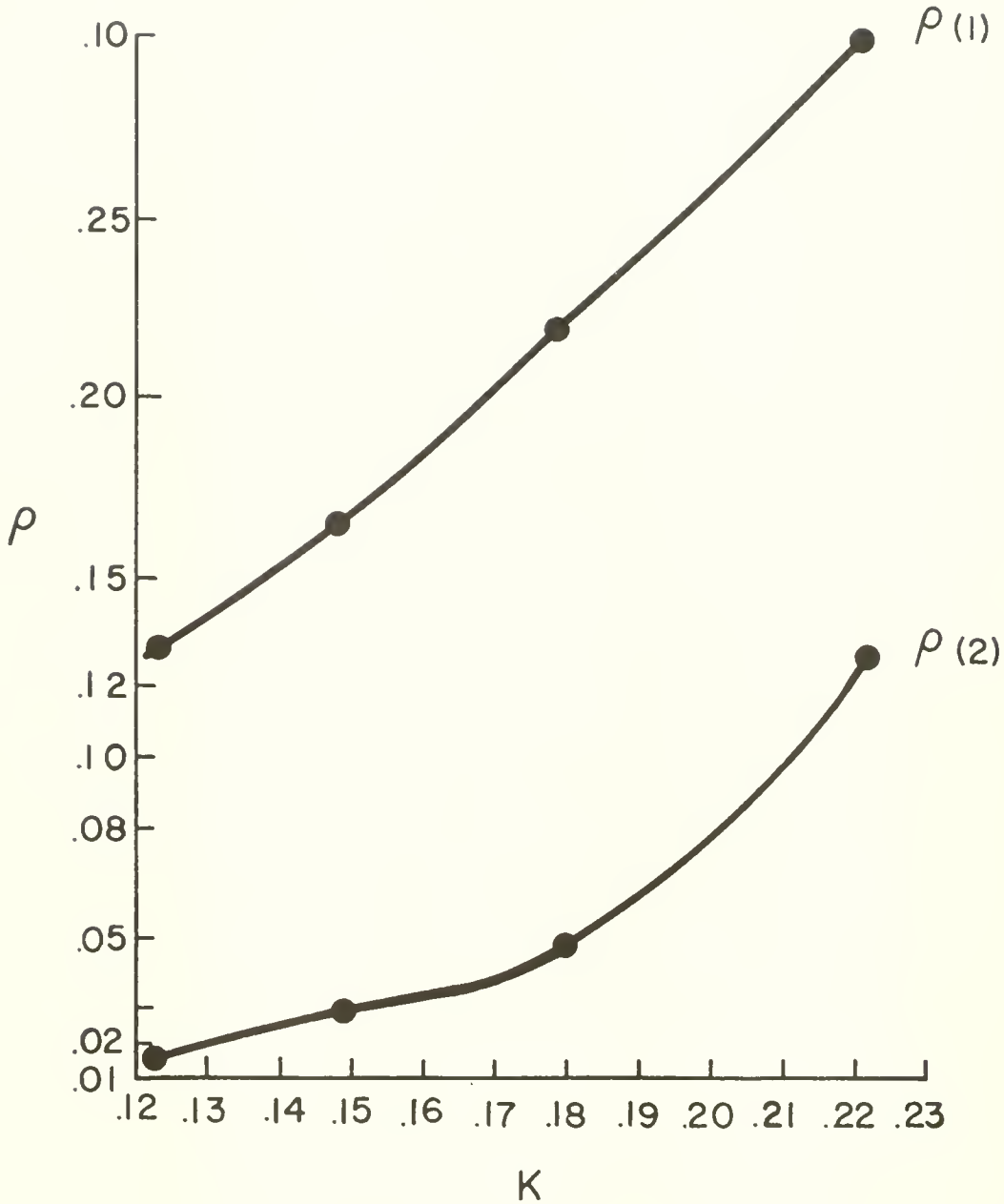


figure 4 Spin Correlation

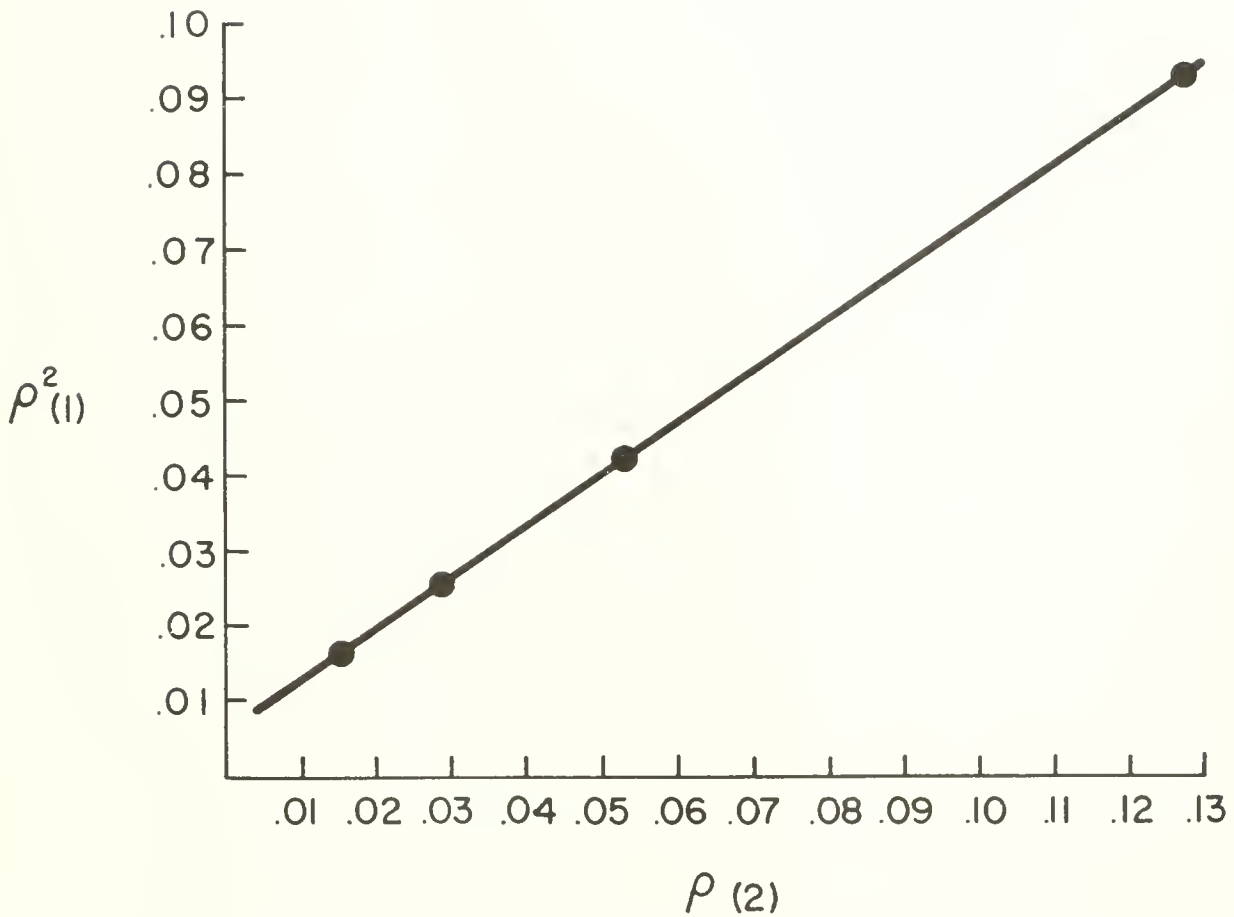

.10
.09
.08
.07
.06
.05
.04
.03
.02
.01
$\rho^2_{(1)}$
.01 .02 .03 .04 .05 .06 .07 .08 .09 .10 .11 .12 .13
$\rho_{(2)}$

figure 5

VII. Conclusions

The significance of the numerical results will now be discussed. The exponential form of the free energy per spin versus lattice size (Figure 1) shows excellent agreement with the result obtained from high temperature graphical analysis, equation (2.42). In Figure 2 it is shown that the low order surface terms dominate the difference in free energies for the lattices with m equal to three and four. However, this is due only to the particular temperature chosen; the surface terms will become more dominant, though smaller, as the temperature is raised. The sample magnetization isotherm (Figure 3) at a temperature above but near the critical temperature shows a large slope (susceptibility) near h = 0. The spin correlations for zero field,

$$\rho(r) = \langle \sigma_i \sigma_{i+r} \rangle ,$$

along the same row (or column) are shown in Figure 4 for r equal to one and two. The range of temperature is from $K_c/1.83$ (high temperature), down to the critical point, K_c. By plotting $\rho^2(1)$ versus $\rho(2)$, Figure 5 suggests exponential behavior which is expected from high temperature graphical expansions.[24]

The Monte Carlo method, using the transfer matrix approach, has been shown to be a successful way of solving large lattice problems. At present, work is being done to test the static

scaling hypotnesis[25] for finite lattices, and to include in the Hamiltonian next nearest neighbor interactions. The first of these tasks will prove the easiest, graphing various magnetization isotherms in terms of reduced variables. The second task, while straightforward, requires a major change in the computer program.

This thesis will conclude with a brief review. Starting from the nearest neighbor Ising Hamiltonian, and using the canonical ensemble, the partition function for a finite lattice was found to be the largest eigenvalue of a matrix called the transfer matrix. The dimensionality of the matrix varied exponentially with the "size" of the lattice. Although the theory was developed in terms of the square lattice of "size" $m \times \infty$, the actual calculations were performed suing the cubic lattice of "size" $m \times m \times \infty$. The largest eigenvalue was shown to be non-degenerate and the corresponding eigenvector contained only non-negative elements. The high temperature power series expansion of the partition function was obtained by graphical techniques. The lowest order difference between the free energy of the bulk lattice (infinite in all directions) and the finite lattice was shown to consist of surface terms whose corresponding graphs circumscribed the lattice.

After introducing the general theory of Monte Carlo, a correspondence was established between the eigenfunction belonging to the largest eigenvalue of the transfer matrix and the steady state collision density of a class of random walks. After choosing a particular random walk, a method of obtaining the

largest eigenvalue was found, which consisted of statistically sampling the walk. Knowledge of the eigenvalue produced the partition function directly, and after an analysis of the bias, produced the free energy. By removing the surface terms from the free energy, and comparing this reduced free energy to the bulk free energy, the effect of the finite size of the lattice was shown. A method of obtaining numerical derivatives of the partition function was found, which consisted of associating a statistical weight to each point in the walk. Using this method both magnetization isotherms and spin correlations were found.

ACKNOWLEDGMENT

I wish to thank Dr. Malvin H. Kalos and Prof. Jerome K. Percus for their help and guidance in the course of this work.

Appendix A. The Branching Process

Proof that the splitting technique, as defined below, produces a random walk whose density is ϕ, where

$$\phi = \frac{BA}{\lambda}\,\phi \tag{A1}$$

λ is the eigenvalue of BA,

A is the stochastic,

B is positive,

and that the mean number of daughters per point is unity. Rules of the walk:

1. Given a point at u' drawn from p.d.f. $\phi_{u'}$, jump it to u by means of the conditional probability $A_{uu'}$.
2. From a density $g_{uu'}(\xi)$, where

$$\langle \xi \rangle = B_{uu'}/\lambda$$

sample a ξ .

3. Split the one parent point into ξ points, each of which remains at u. For example, if $\xi = 3$, the single point at u becomes three points at u.

In any random process, the mean number of outcomes of an event ℓ equals the number of trials times the probability of the outcome ℓ. For example, the mean number of heads in N flips of a coin is N/2. Using this principle, consider N points in a population, the position u of each drawn from density ϕ_u.

Move each point independently according to the above rules. Let:

$C(u')$ be the mean number at u' before the move.

$J(u,u')$ be the mean fraction of these moving to u.

$D(u,u')$ be the mean number of daughters created per arrival at u from u'.

$M(u,u')$ be the mean number arriving at u from u'.

Then,

$$M(u,u') = D(u,u')J(u,u')C(u') \quad . \tag{A2}$$

Let $M(u)$ be the mean number arriving at u from any u'.

$$M(u) = \sum_{u'} M(u,u') = \sum_{u'} D(u)J(u,u')C(u') \quad . \tag{A3}$$

But, by definition,

$$D(u,u') \equiv B_{uu'}/\lambda \quad ; \tag{A4}$$

also

$$C(u') = N\phi_{u'} \tag{A5}$$

N being the population size before the jump, and

$$J(u,u') = A_{uu'}$$

Therefore, comparing equation (A3) with equation (A1),

$$M(u) = N\phi_u \quad ,$$

proving that the population stochastically duplicates itself after the moves. Since by definition ϕ is normalized,

(A8) $$\sum_u \phi_u = 1 \quad ,$$

the mean number of points ($\bar{N}$) after the jump equals the number of points before the jump (N), since

(A9) $$\bar{N} = \sum_u M(u) = \sum_u N\phi_u = N \quad .$$

Therefore, the use of the correct eigenvalue λ stabilizes the population. This fact is used to provide a Monte Carlo estimator of λ .

Appendix B. The Mean and Variance of a Lognormal Estimator.

Let X_E be a random variable with normal density:

$$(B1) \qquad P(X_E) = \frac{1}{\sqrt{2\pi Q^2_{X_E}}} \exp\left[\frac{-(X_E-X)^2}{2Q^2_{X_E}}\right] ,$$

where $Q^2_{X_E}$ is the variance.

Expand $\ell n\ X_E$ in a Taylor series about X:

$$(B2) \quad \ell n\ X_E = \ell n\ X + \frac{1}{X}(X_E-X) - \frac{1}{2X^2}(X_E-X)^2 + \frac{1}{3X^3}(X_E-X)^3 - O[(X_E-X)^4] .$$

Take the mean of $\ell n\ X_E$ over the normal distribution:

$$(B3) \qquad M(\ell n\ X_E) = \int \ell n\ X_E\ P(X_E)dX_E .$$

Substituting the expansion for $\ell n\ X_E$,

$$(B4) \quad M(\ell n\ X_E) = \ell n\ X - \frac{1}{2X^2}\int (X_E-X)^2 P(X_E)dX_E .$$

The second and fourth terms in the expansion give zero contribution. Therefore,

$$(B5) \qquad M(\ell n\ X_E) = \ell n\ X - \frac{Q^2_{X_E}}{2X^2}$$

proving that $\ell n\ X_E$ is a biased estimator of $\ell n\ X$, with bias B,

$$(B6) \qquad B = \frac{Q^2_{X_E}}{2X^2}$$

to fourth order.

The variance of $\ell n\ X_E$ may be similarly obtained. Expand $\ell n^2 X_E$:

$$(B7)\quad \ell n^2 X_E = \ell n^2 X + \frac{2\ell n\ X}{X}(X_E - X) + \left[\frac{2}{X^2} - \frac{2\ell n\ X}{X^2}\right] \frac{(X_E - X)^2}{2}$$

Again, the first and third order terms give zero contribution:

$$(B8)\qquad M(\ell n^2 X_E) = \ell n^2 X + \frac{Q_{X_E}^2}{X^2} - \frac{Q_{X_E}^2\ \ell n\ X}{X^2}$$

Now,

$$(B9)\qquad V(\ell n\ X_E) = M(\ell n^2 X_E) - [M(\ell n\ X_E)]^2$$

where V is the variance.

$$(B10)\quad V(\ell n\ X_E) = \ell n^2 X - \frac{Q_{X_E}^2}{X^2} - \frac{Q_{X_E}^2\ \ell n\ X}{X^2} - \left[\ell n^2 X - \frac{Q_{X_E}^2\ \ell n\ X}{X^2} + O\left(\frac{Q_{X_E}^4}{X^4}\right)\right])$$

so that

$$(B11)\qquad V(\ell n\ X_E) = \frac{Q_{X_E}^2}{X^2}$$

or

$$(B12)\qquad \sigma_{\ell n\ X_E} = \frac{Q_{X_E}}{X}$$

For any estimator, X_E, worthy of the name, and in particular for the results in this thesis,

$$\frac{Q_{X_E}}{X} < 1 \; ; \tag{B13}$$

but, from equation (B6),

$$B = \frac{1}{2} \sigma^2_{\ell n\ \lambda_E} << \sigma_{\ell n\ \lambda_E} \tag{B14}$$

for any good estimator. Therefore, the bias of the estimator, $\ell n\ \lambda_E$, is so much smaller than the measure of statistical error, $\sigma_{\ell n\ E}$, that it can be neglected.

Appendix C. Magnetization and Spin Correlation.

To obtain both the magnetization and the spin correlation, logarithmic derivatives of the free energy are needed. From equation (1.15), the magnetization per spin is

$$M(h) = \frac{1}{N}\frac{\partial \ln Z}{\partial h} = \frac{1}{m}\frac{\partial \ln \lambda}{\partial h} \quad , \tag{C1}$$

where, as previously, the square lattice is being considered for convenience of notation.

The spin correlation may be defined as

$$\rho(r) = \langle \sigma_i, \sigma_{i+r} \rangle \tag{C2}$$

for two spins in the same layer, separated by a "distance" r. This function can be put in the form of a logarithmic derivative of the free energy by means of the following technique. In each layer of the lattice, create a coupling between spin i and spin i+r. That is, add to the Hamiltonian the term

$$-k_B T L \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i+r,j} \tag{C3}$$

where i is the intralayer index and j is the interlayer index. The new Hamiltonian becomes

$$\mathcal{H}' = \mathcal{H}_I - k_B T L \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i+L,j} \tag{C4}$$

then,

$$(C5) \qquad Z' = \sum_{u_1,u_2\ldots u_n} \exp\left[\frac{\mathcal{H}_I}{k_B T}\right] \exp\left[\sum_{j=1}^{n} L\sigma_{i,j}\sigma_{i+r,j}\right]$$

and

$$(C6) \qquad \left.\frac{\partial \ \ell n\ Z'}{\partial L}\right|_{L=0} = \left\langle \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i+r,j} \right\rangle,$$

where the average is for the standard Ising lattice. Using the translational symmetry of the lattice,

$$(C7) \qquad \left\langle \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i+r,j} \right\rangle = n\left\langle \sigma_i,\sigma_{i+r} \right\rangle$$

and

$$(C8) \qquad \rho(r) = \frac{1}{n} \left.\frac{\partial \ \ell n\ Z'}{\partial L}\right|_{L=0} \quad)$$

producing the result

$$(C9) \qquad \rho(r) = \left.\frac{\partial \ \ell n\ \lambda}{\partial L}\right|_{L=0}$$

Since both M(h) and $\rho(r)$ are logarithmic derivatives of the free energy, the Monte Carlo methods of solution will be developed in terms of the magnetization.

Using the finite difference approximation

$$(C10) \qquad M(h) \simeq \frac{1}{m}\left[\frac{\ell n\ \lambda(h+\Delta h) - \ell n\ \lambda(h)}{\Delta h}\right]$$

and assuming that both $\ell n\ \lambda(h+\Delta)$ and $\ell n\ \lambda(h)$ are exactly known, the error involved is negligible, because $\ell n\ \lambda$ is a smooth function of h away from the critical point, and Δh will be of order 10^{-7}.

In standard numerical procedures, use of the finite difference approximation should be avoided if possible because any small error in either $\ell n\ \lambda(h+\Delta)$ or $\lambda(h)$ produces a large error in the finite difference derivative. In fact, this error gets larger as Δh gets smaller. Fortunately, Monte Carlo avoids this problem. If the Monte Carlo estimate of $\ell n\ \lambda(h+\Delta h)$ is highly correlated with the estimate of $\ell n\ \lambda(h)$, any error in one will, with high probability, occur in the other and will cancel in the difference, $\ell n\ \lambda(h+\Delta) - \ell n\ \lambda(h)$.

This correlation was produced by the use of statistical weights, which will now be described. After stability has been reached, associate with each point (i) in the population a number w_i. Set each w_i equal to 1. Iterate the population in the standard fashion,

$$\vec{\Psi}(h) = \frac{V_3(h)V_2V_1}{\lambda}\,\vec{\Psi}(h) \quad , \tag{C11}$$

where the dependence on h is shown explicitly. After each point moves from its old position, u' , to its new position, u multiply the point's weight by

$$\left\langle u\right| \frac{V_3(h+\Delta h)}{V_3(h)} \left|u\right\rangle \tag{C12}$$

i.e.,

$$w_i = w_i \left\langle u \left| \frac{V_3(h+\Delta h)}{V_3(h)} \right| u \right\rangle . \tag{C13}$$

After fissioning the point, associate this new weight with each of its daughters.

After the iteration, the particle density is, as usual, $\vec{\Psi}(h)$. However, the weight density is $\vec{\Psi}(h+\Delta h)$, as will now be shown. Let the mean arrival of weight at u be $\vec{\chi}$. Then,

$$\chi_u = \sum_{u'} \left(\frac{V_3(h+\Delta h)}{V_3(h)} \right)_{uu} \frac{(V_3(h))_{uu} (V_2)_{uu} (V_1)_{uu'}}{\lambda} \chi_{u'} . \tag{C14}$$

In words:

> The mean arrival of weight at u, χ_u, equals the mean weight at u', $\chi_{u'}$, times the mean fraction moving from u' to u, times the mean number of daughters per point, times the number
>
> $$\left[\frac{V_3(h+\Delta h)}{V_3(h)} \right]_{uu} \tag{C15}$$
>
> summed over all u'.

Simplifying,

$$\chi_u = \sum_{u'} (V_3(h+\Delta h))_{uu} \frac{(V_2)_{uu} (V_1)_{uu'}}{\lambda} \chi_{u'} \tag{C16}$$

But this is the equation satisfied by $(h+\Delta h)$. Therefore,

$$\vec{\chi} = \vec{\Psi}(h+\Delta h) . \tag{C17}$$

The result is that the bare points are distributed according to $\vec{\Psi}(h)$, and the same points with associated weights are distributed according to $\vec{\Psi}(h+\Delta h)$.

The difference in equation (C10) which must be estimated is

$$R = \ell n\ \lambda(h+\Delta h) - \ell n\ \lambda(h) \ . \tag{C18}$$

To estimate $\ell n\ \lambda(h)$, equation (4.56) was used. The estimator of $\ell n\ \lambda(h+\Delta h)$ is just an extension of equation (4.54) to the case of weighted points:

$$\ell n\ \lambda(h+\Delta h)_{EST} = \ell n\ \lambda_T + \ell n \left[\frac{\langle W_A \rangle}{W_B} \right]_{EST} , \tag{C19}$$

where

W_A = sum of the weights after the iteration,

W_B = sum of the weights before the iteration.

Sample magnetization and correlation curves are contained in Section VI.

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